

INTERFACE BY DESIGN FOR JOINING OF DISSIMILAR MATERIALS

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Project ID #
mat136

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OVERVIEW

Timeline

- ▶ State date:
 - October 1, 2017
- ▶ End date:
 - September 30, 2020
- ▶ 85% complete

Budget

- ▶ Total project funding
 - DOE share: \$2,825k
 - Contractor share: \$0
- ▶ Funding for FY 2019: \$900K
- ▶ Funding for FY 2020: \$1,025K
 - \$500K/year at ORNL
 - \$400K/year at PNNL
 - \$125k/year at ANL

Barriers

- ▶ Lack of reliable joining methods for dissimilar materials
- ▶ Lack of fundamental understandings on the bond formation mechanisms at the interface
- ▶ 2017 U.S. DRIVE MTT Roadmap Report, section 4

Partners

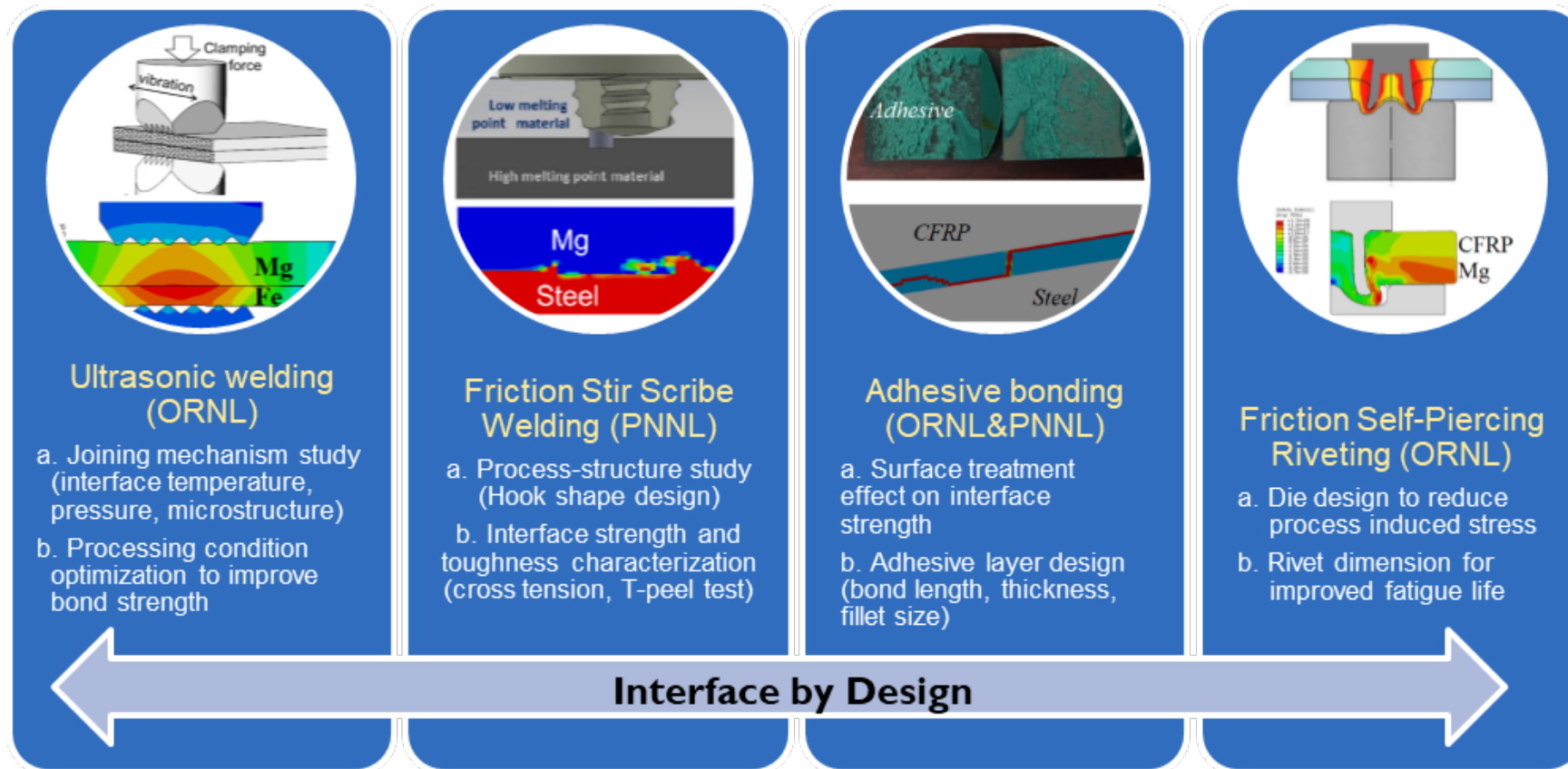
- ▶ ORNL/PNNL/ANL
- ▶ Industry collaborations through materials supply and technical advisory committee

RELEVANCE AND IMPACT

- ▶ Technology gaps for lightweight metal body structures
 - Lack of proven technology for joining dissimilar metals (Steel-Al, Steel-Mg, Mg-Al, etc.)
 - The need to maintain the microstructure makes the use of conventional joining techniques nearly impossible.
 - Joining of thin sheet of AHSS is unreliable and fracture behavior is not understood.
- ▶ Technology Gaps-Composite Body Structures
 - Lack of dependable joining technology for the integration of composite components into the body structure



INTERFACE BY DESIGN FOR VARIOUS MATERIAL PROCESSING PROJECT

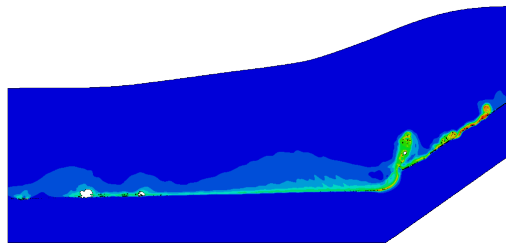


Geometric factor, intrinsic strength, interface morphology, tool design

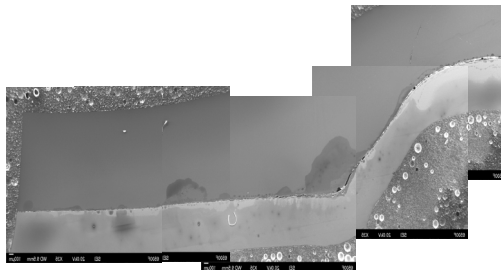
TECHNICAL APPROACH

Interface-by-design Framework

Macroscopic process
simulation (FE)



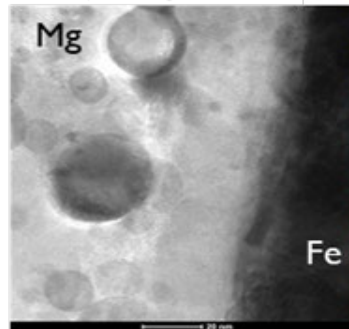
Process simulation of Mg/steel
impact welding



SEM of Mg/steel impact joint

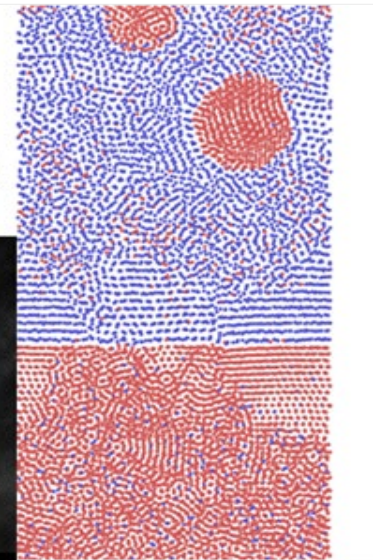
Diffusion
(DICTRA/MD)

↑T ↑V
Mechanical mixing.
Formation of Fe
particles and SRO.
EXP: Impact welding
with jet layer

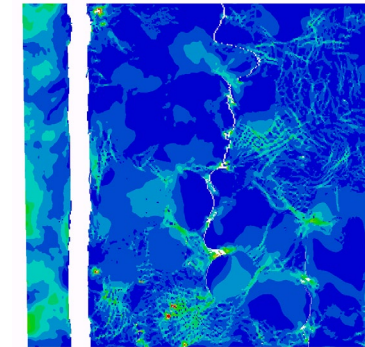


High bonding strength due to SRO-
induced low misfit strain energy at
interface

Microstructure
(Thermo-Calc &
phase field)



Microstructural
mechanical
simulation

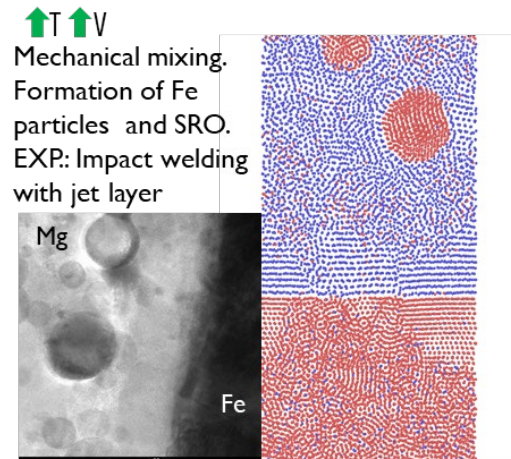
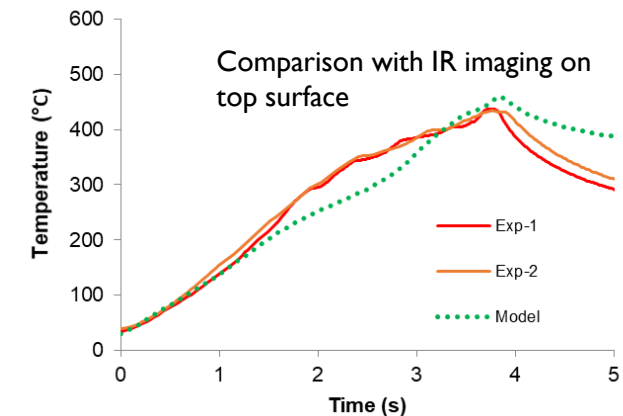
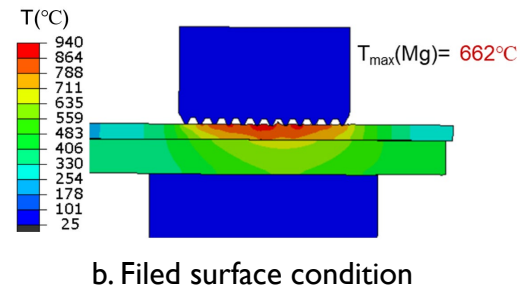
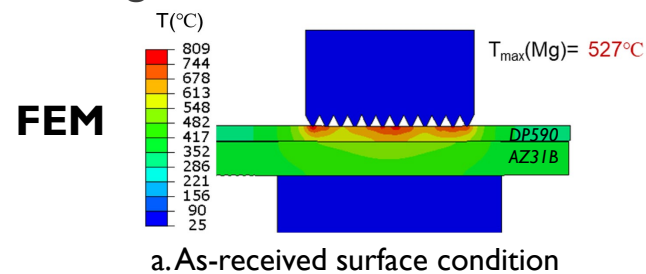


Validation via
mechanical test: failure
load and fracture
surface measurements

FY18-19 ACCOMPLISHMENTS ON MG/FE INTERFACE

ORNL -- VALIDATED PROCESS SIMULATION LINKING PROCESS-INTERFACIAL STRUCTURES- JOINT PROPERTIES

- Developed and demonstrated Interface-by-Design framework by creating metallurgical bond between Mg and uncoated steel with ultrasonic and impact welding through process simulation, interface formation simulation and welding trials



High bonding strength due to SRO-induced low misfit strain energy at interface

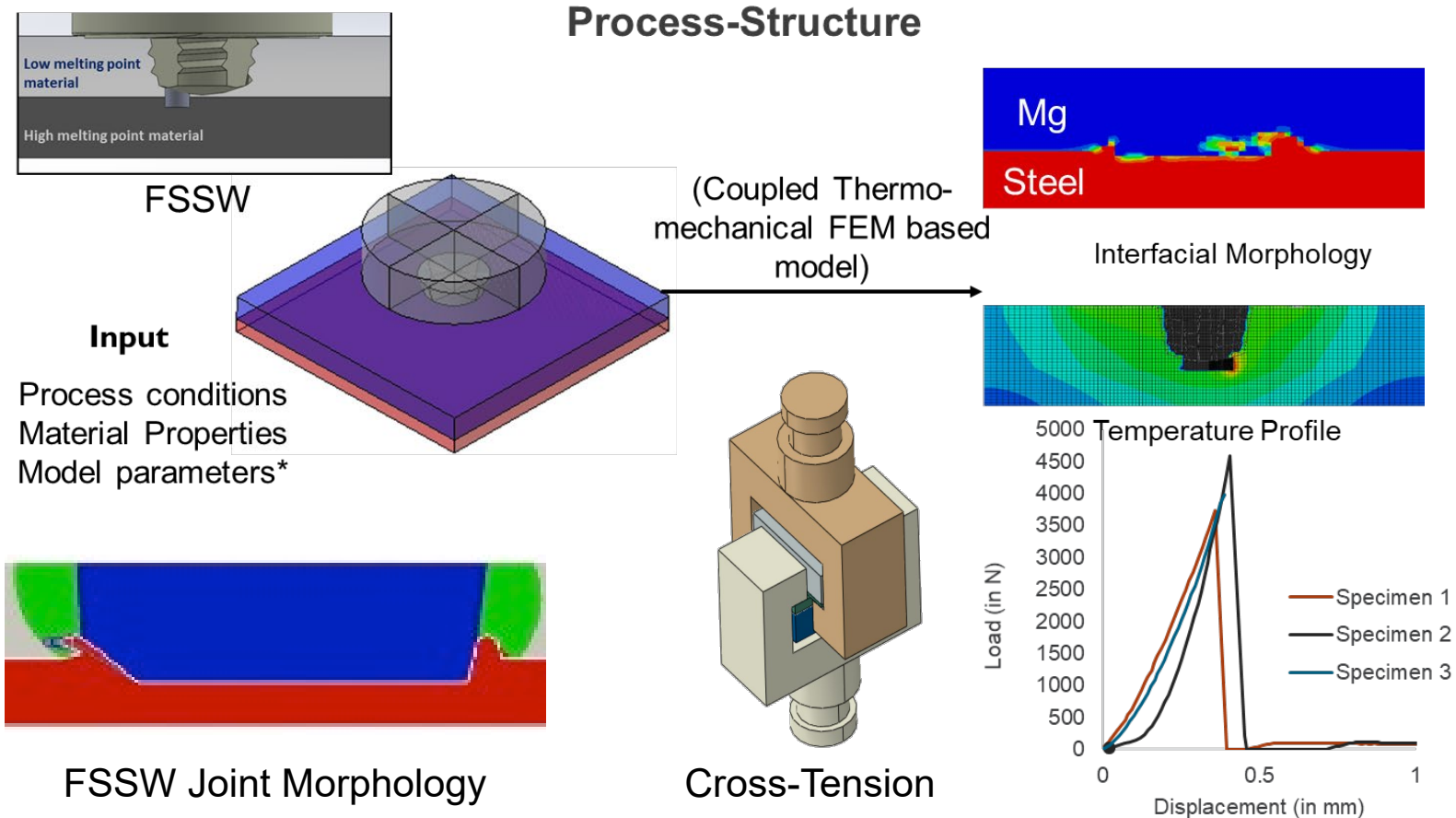
Comparison of joint strength between different welding and surface conditions

Surfs condition Case	Faying surface	Other surfaces	Welding Power and time	Condition	Tensile load
0	Sanded P80 (Mg)	As received	2500 W, 2 s	Baseline	Fail drop test
1	Sanded P80 (Mg)	As received	3500 W, 2 s	Increased velocity	Pass drop test
2	Sanded P80 (Mg)	As received	3500 W, 4 s	Increased welding time	3.9±0.5 kN
3	Filed	Filed	3500 W, 4 s	Surface modification	4.2±0.4kN

FY18-19 ACCOMPLISHMENTS ON MG/FE INTERFACE

PNNL -- VALIDATED PROCESS SIMULATION LINKING PROCESS-INTERFACIAL STRUCTURES- JOINT PROPERTIES

- Developed and demonstrated Interface-by-Design framework by creating metallurgical bond between *Mg and uncoated steel* with friction stir scribe welding through process simulation, interface formation simulation and welding trials



FY20 MILESTONES, PROGRESS AND ACCOMPLISHMENTS

-- FOCUSING ON MG- COATED STEEL INTERFACE

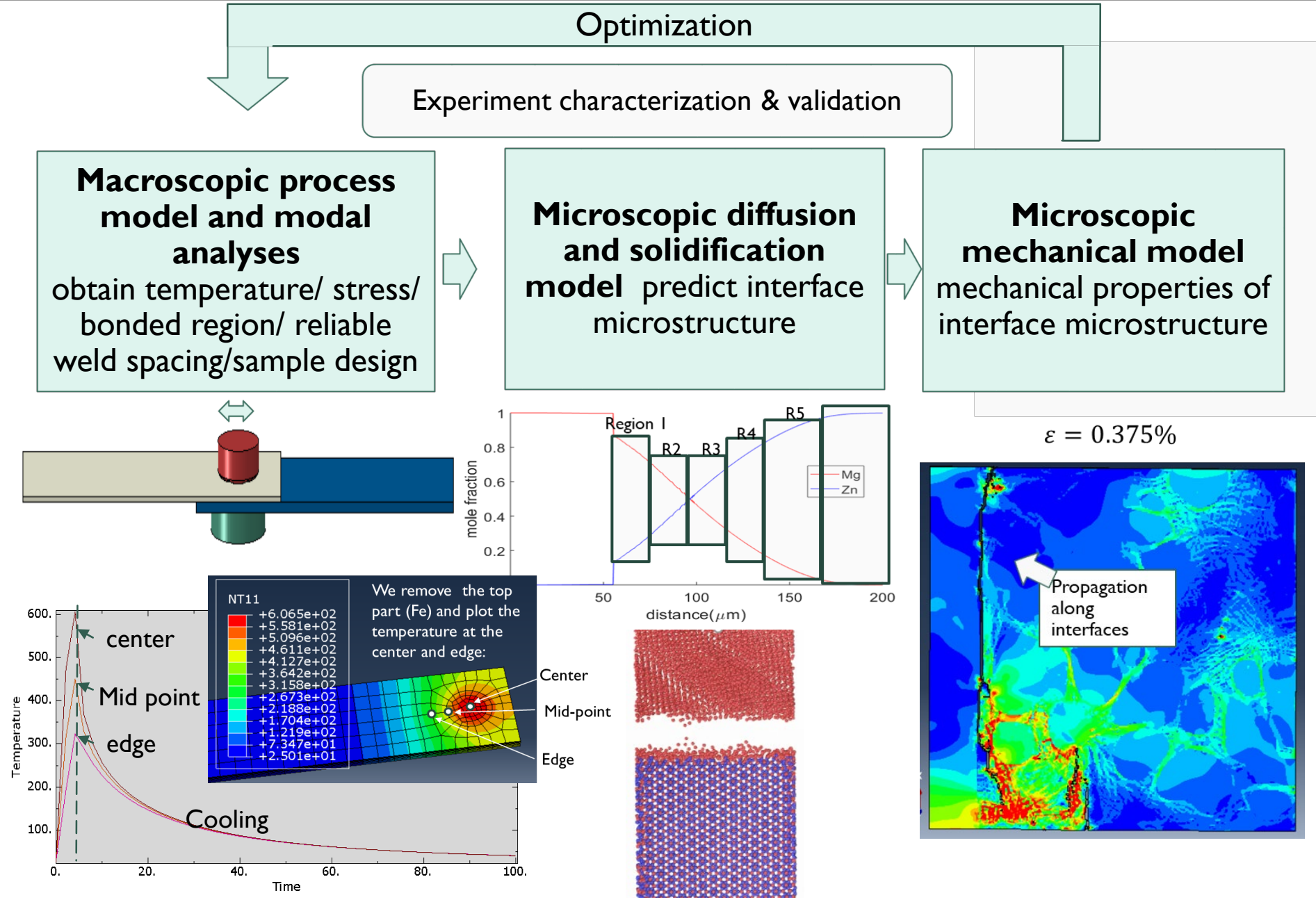
FY20 Milestones

- ORNL -- Demonstrate the interface by design framework in producing structural joints of Mg to coated high strength steel
- PNNL -- Obtain and validate the adhesive parameters for an adhesive joint from the combined experimental and computational framework

FY20 Progress and Accomplishments

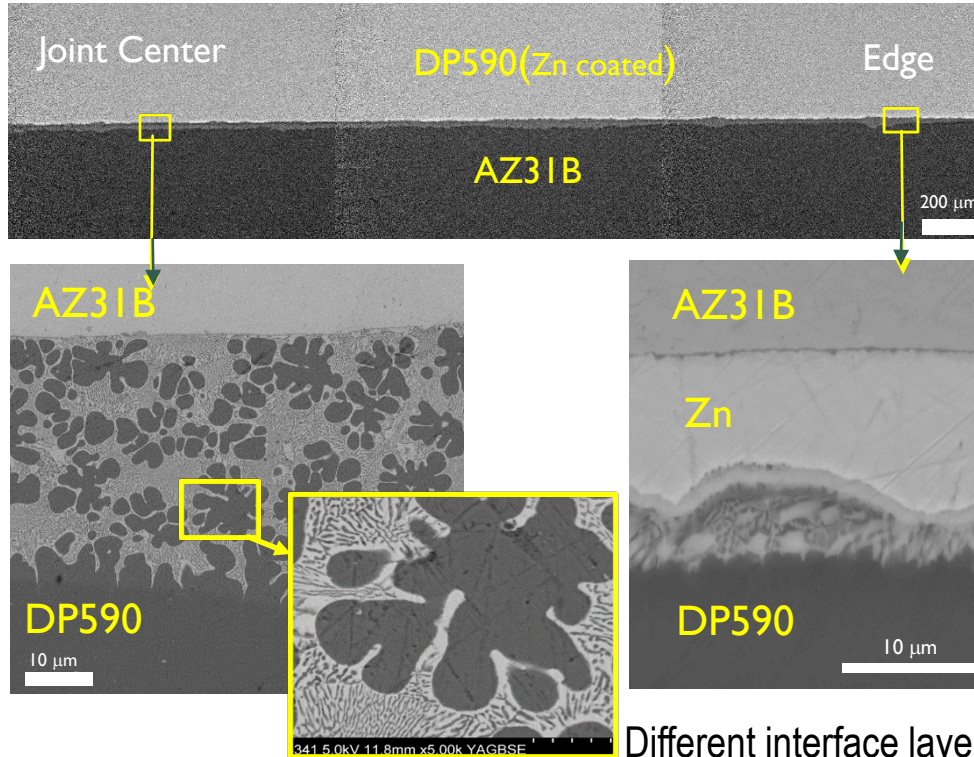
- ORNL:
 - Developed and validated forward prediction framework for Mg-coated steel interface with ultrasonic welding
 - Developed modal analyses framework to enable reliable ultrasonic weld coupon design
- PNNL:
 - Combined modeling and experimental effort to standardize test configurations for mechanical characterization of the joints interface
 - Developed an integrated DIC ZFEM framework to inversely identify joints characteristics

FY20 ORNL -- A predictive framework to link USW process parameters to Mg/coated steel interface mechanical properties - Guiding process design and optimization



Multi-modal joint interface microstructure characterization

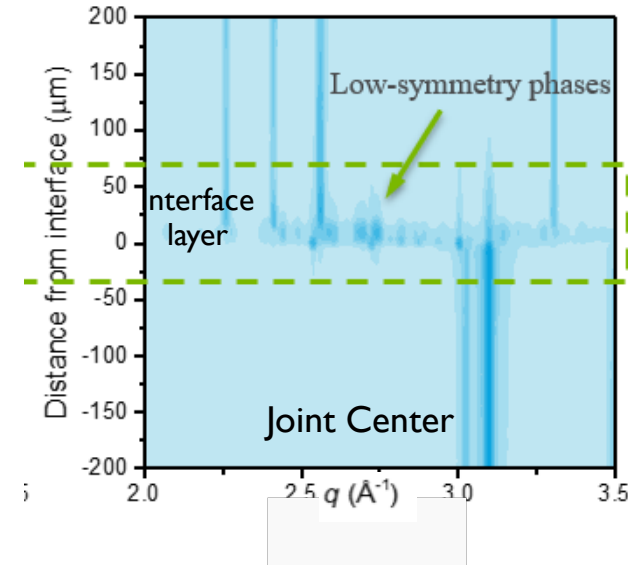
SEM (ORNL) result shows various microstructure at different locations of Mg/coated steel USW joint interface



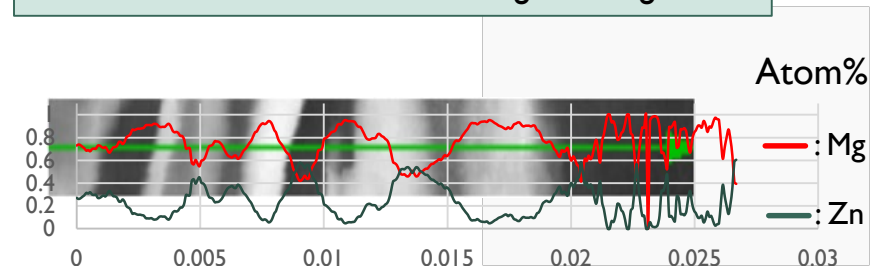
Uniform interlayer of Mg dendrite and eutectic microstructure at the joint center

Different interface layers with different compositions at the joint edge

Synchrotron X-ray (ANL) helps to reveal the intermetallic phases at joint interface



STEM-EDXS line scan identifies the (center) eutectic microstructure is Mg and MgZn

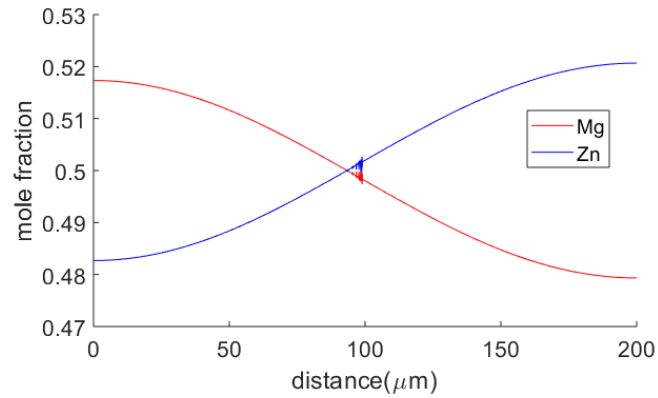


Provided experimental validation for the establishment of robust computational tool to link process parameters to different interface microstructures and macroscopic strength

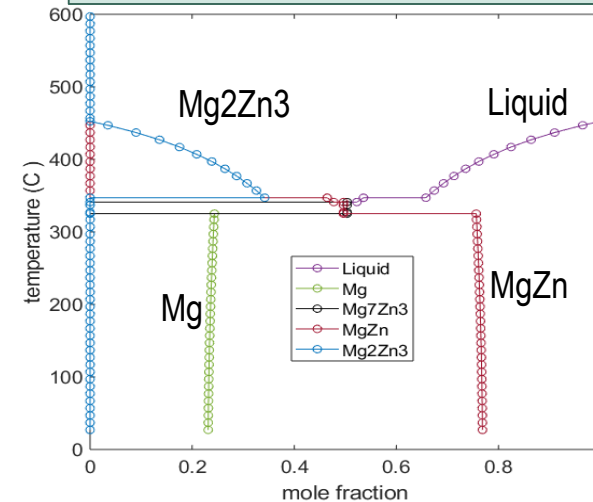
Microscopic diffusion and solidification model to predict interfacial microstructure

- Based on temperature history, interfacial diffusion at different location is predicted using DICTRA
- With diffusion result and cooling rate, solidification microstructure is predicted using Thermo-Calc
- Phase field model is next used to predict the microstructure morphology upon cooling (ongoing)

Uniform diffusion result predicted in center

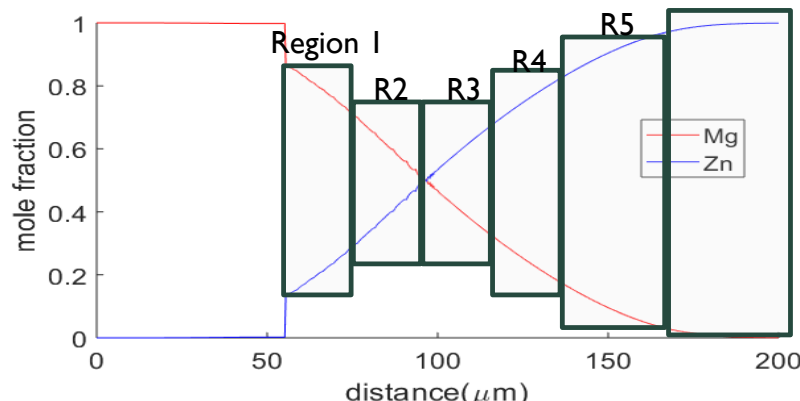


Thermo-Calc prediction of solidification (center)



Predicted final microstructure consists of Mg and MgZn, which is consistent with STEM-EDXS result

Layered interface structure predicted on edge



Thermo-Calc prediction on each layer (edge)

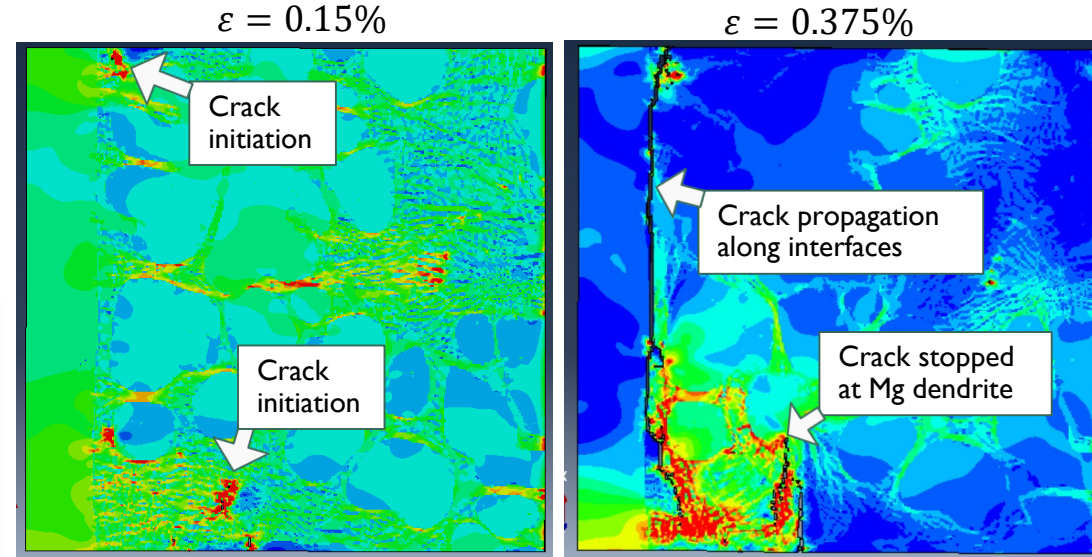
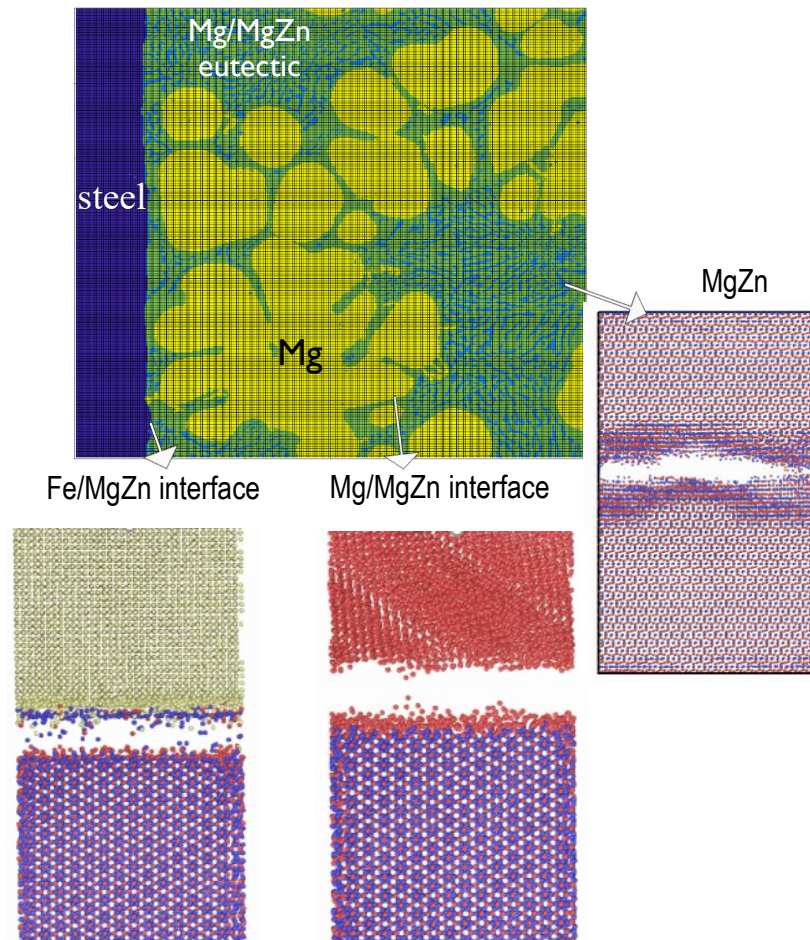
- Region 1: 64% Mg_7Zn_3 34% Mg 2% MgZn
 Region 2: 62% Mg_7Zn_3 33% Mg_2Zn_3 5% MgZn
 Region 3: 100% Mg_2Zn_3
 Region 4: 81% $\text{Mg}_2\text{Zn}_{11}$ 19% Mg_2Zn_3
 Region 5: 64% $\text{Mg}_2\text{Zn}_{11}$ 36% Zn
 Region 6: 100% Zn

Microstructure-based FE model predicts joint strength and failure mode

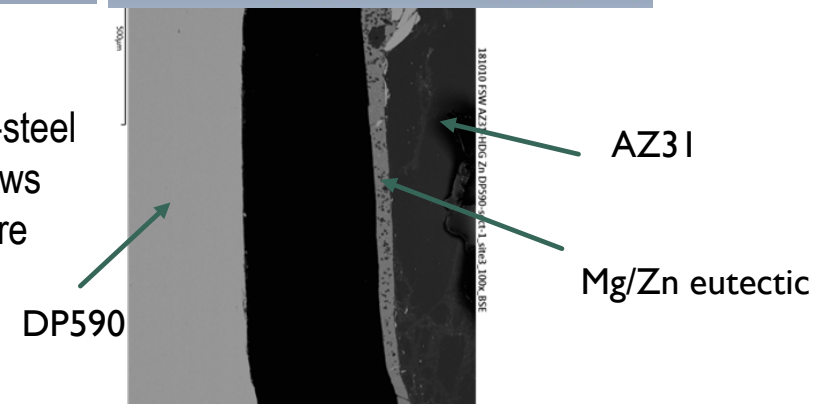
- Microstructure-based FE model of joint interface is developed for prediction of joint performance
- Same methodology will be used for different microstructure obtained from other process parameters, generating data for optimization

Microstructure-based model contains Mg, MgZn, steel phases and their interfaces, properties informed by MD simulations

Simulation shows stress concentration in eutectic phase triggers crack initiation, and propagation along eutectic-steel interface



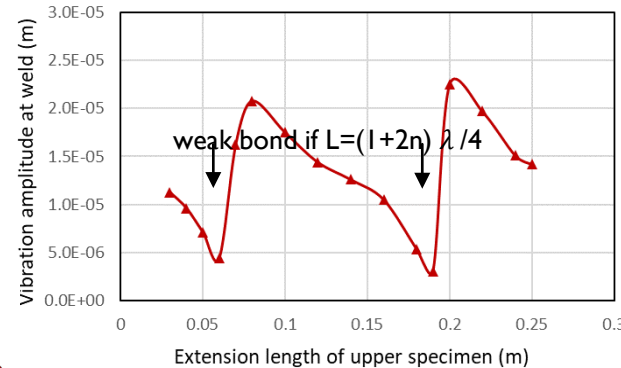
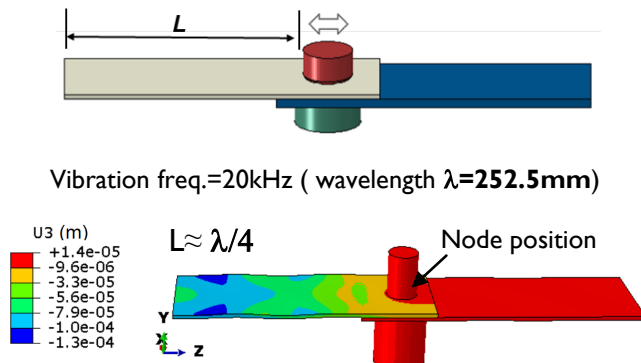
Fractography (SEM) of Mg-steel friction stir welded joint shows consistent result that fracture breaks steel-eutectic layer interface (PNNL)



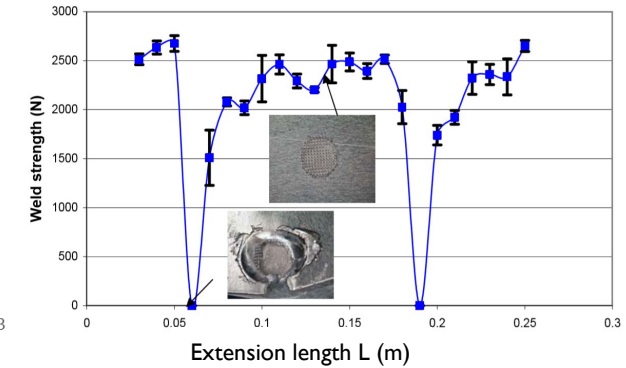
Modal Analysis Linking Sample Design to Joint Quality for USW

USW joint quality is known to be sensitive to processing condition and sheet dimension: A modal analysis tool is developed to compute global motion and stress distribution for reliable weld spacing and coupon design.

Al-6061 USW – Effect of coupon length

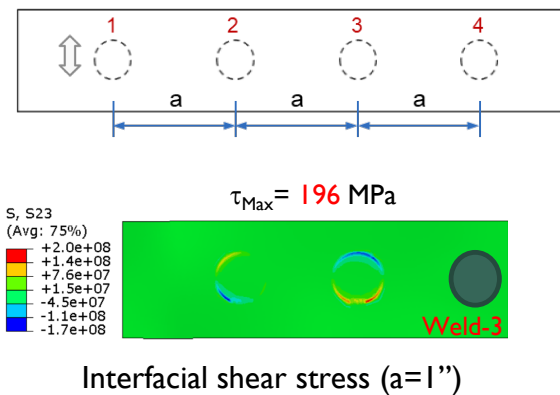


Predicted interfacial relative vibration

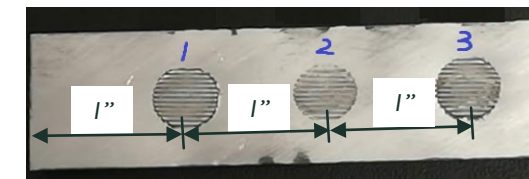
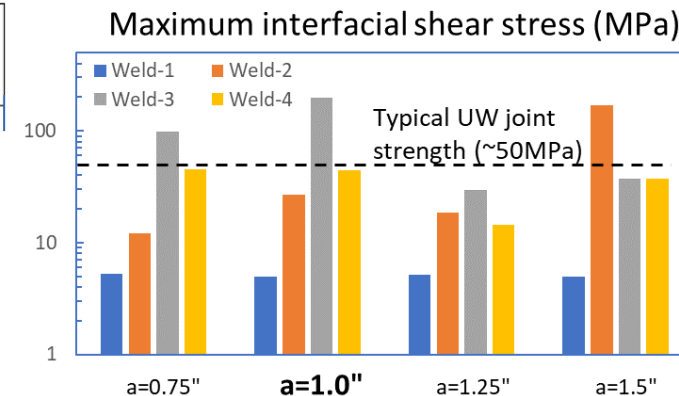


Measured joint strength by de Vries E.

AZ31 USW weld design – Effect of weld spacing



Interfacial shear stress ($a=1''$)



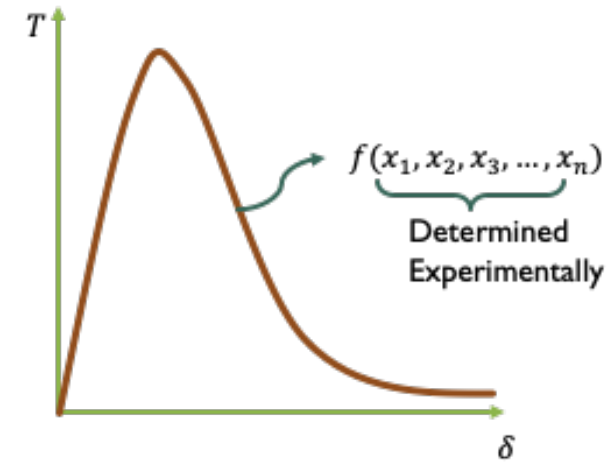
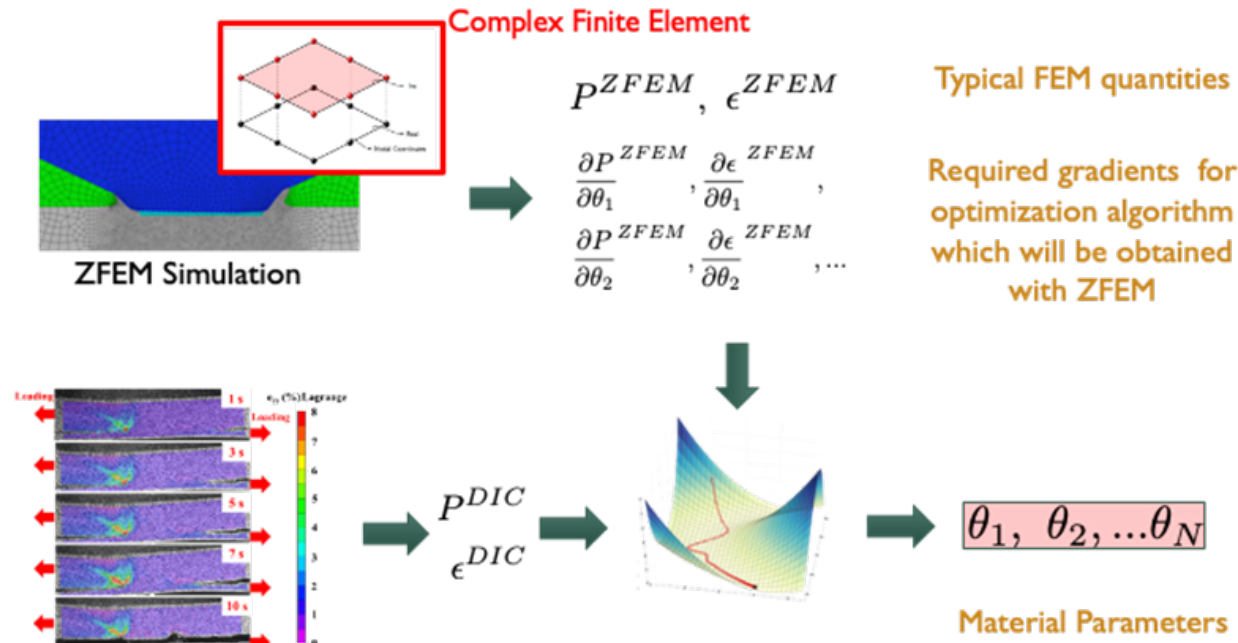
Weld-1 and Weld-2 failed when joining Weld-3.

FY20 PNNL ACCOMPLISHMENTS MG/STEEL INTERFACE

-- NOVEL INVERSE FE-BASED INTEGRATED DIC APPROACH

Motivation:

- For finite element (FE) simulations of joint performance, a requirement is the availability of the model parameters governing the interface.
- Experiments required are difficult and expensive; still rely on non-unique calibrations and lots of assumptions.
- An inverse FE approach does not have test geometry restrictions.
- Allows for quantitative use of Digital Image Correlation (DIC) data from a mechanical test.

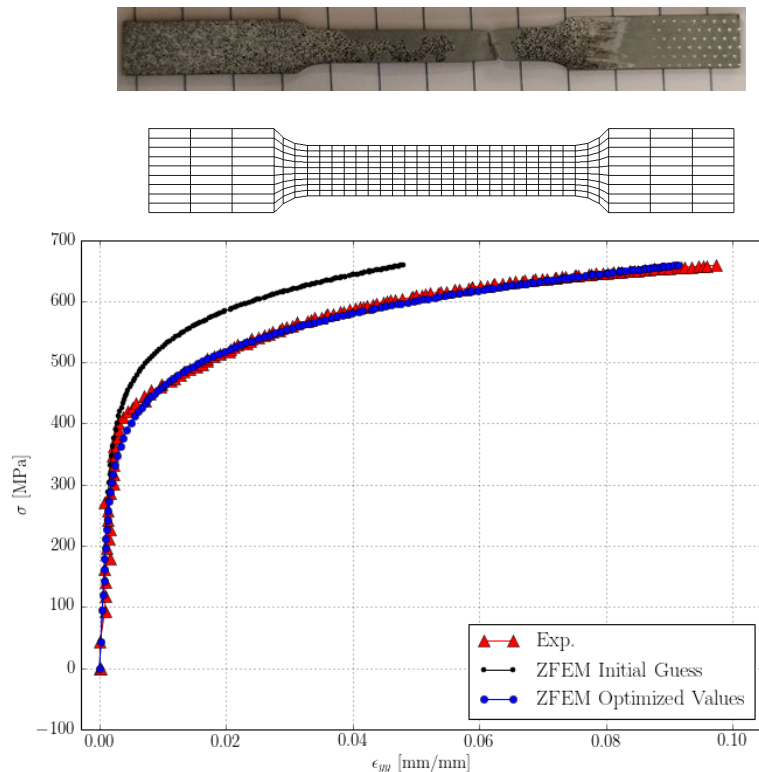


Load displacement curve from experiment

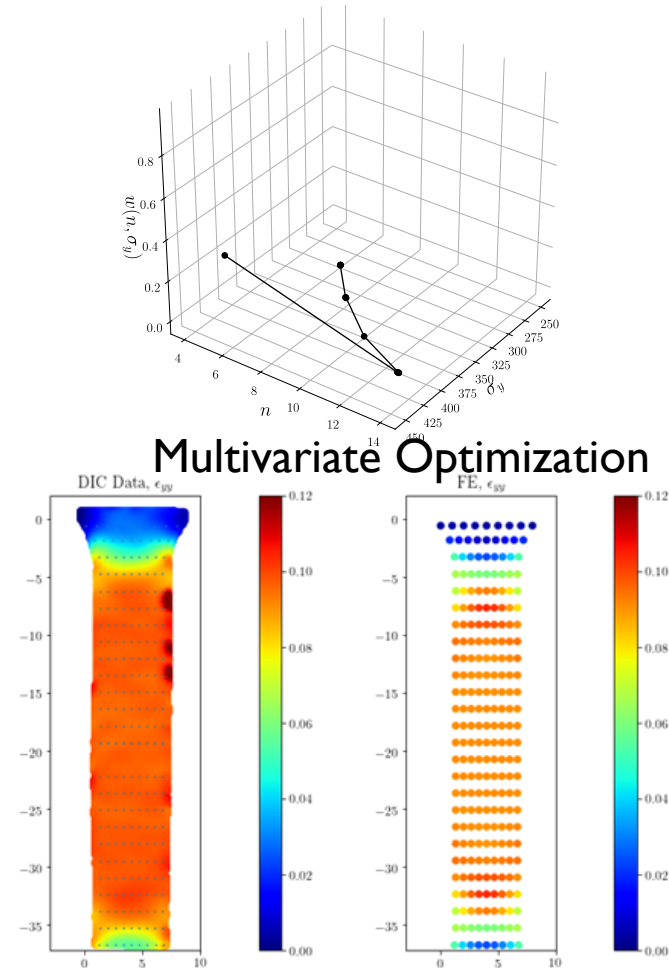
FY20 ACCOMPLISHMENTS ON MG/STEEL INTERFACE

-- VALIDATION EXAMPLE/TENSILE TEST

- Tensile test example is solved for validating the optimization algorithm.



Results: SS curve



Contour plots. DIC vs FEM.

σ_y [MPa]	n
380	8
379.91	9.765
379.90	9.884
379.64	9.889
379.55	9.8504
341.01	7.665
340.63	7.6749
338.59	7.6091
323.26	6.8813
322.5832	6.8542
322.5822	6.8801
322.5819	6.8849
322.5817	6.8857

Optimized Values

FY20 ACCOMPLISHMENTS ON MG/STEEL INTERFACE

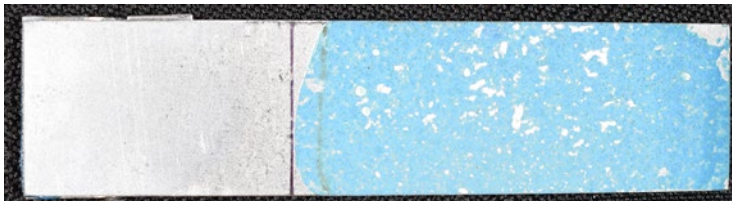
-- EXPERIMENTAL DATA-- DCB TEST

- Double cantilever beam test for adhesively bonded steel plates.

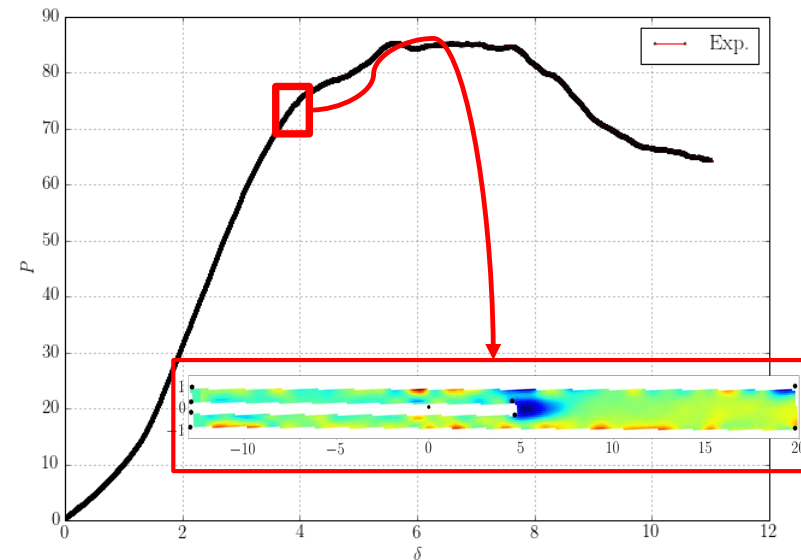
Experimental Set-up



Image of fractured sample showing the location of adhesive:



- Time, reaction force, displacement at each time step



- Full-field DIC data for each time step including displacement and strain fields

FY20 ACCOMPLISHMENTS ON MG/STEEL INTERFACE

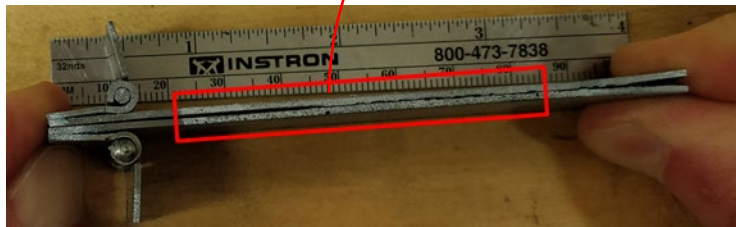
-- DIC REGION OF INTEREST AND FINITE ELEMENT MODEL

Reference point marked by white square.
Corresponds to start of bond line.



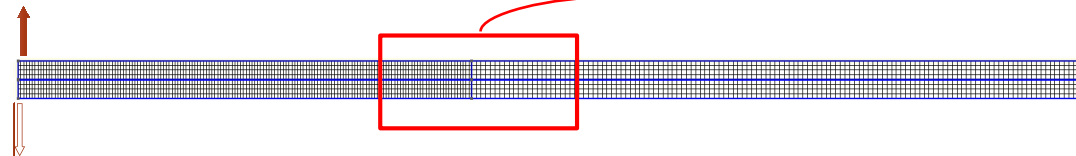
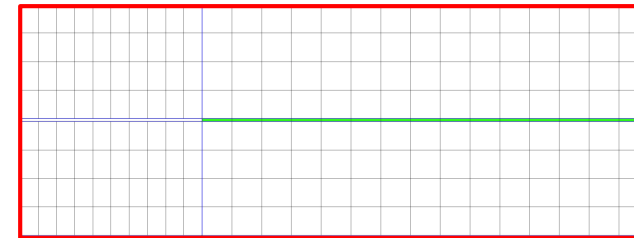
DIC Result

Region of interest



Experimental Set-Up

Layer of zero
thickness cohesive
elements (green)



Finite Element Model with a layer of cohesive elements

FY20 ACCOMPLISHMENTS ON MG/STEEL INTERFACE

-- SIMULATION VS EXPERIMENTAL RESULTS

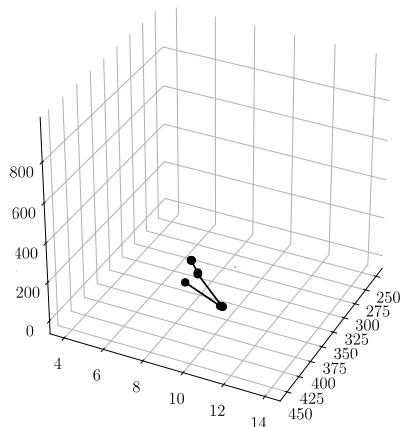
- Starting with an initial guess for the joint parameters, multiple FE simulation iterations are performed with the objective of minimizing residual quantity (discrepancy between the DIC data and the FE simulation results)

Initial guess

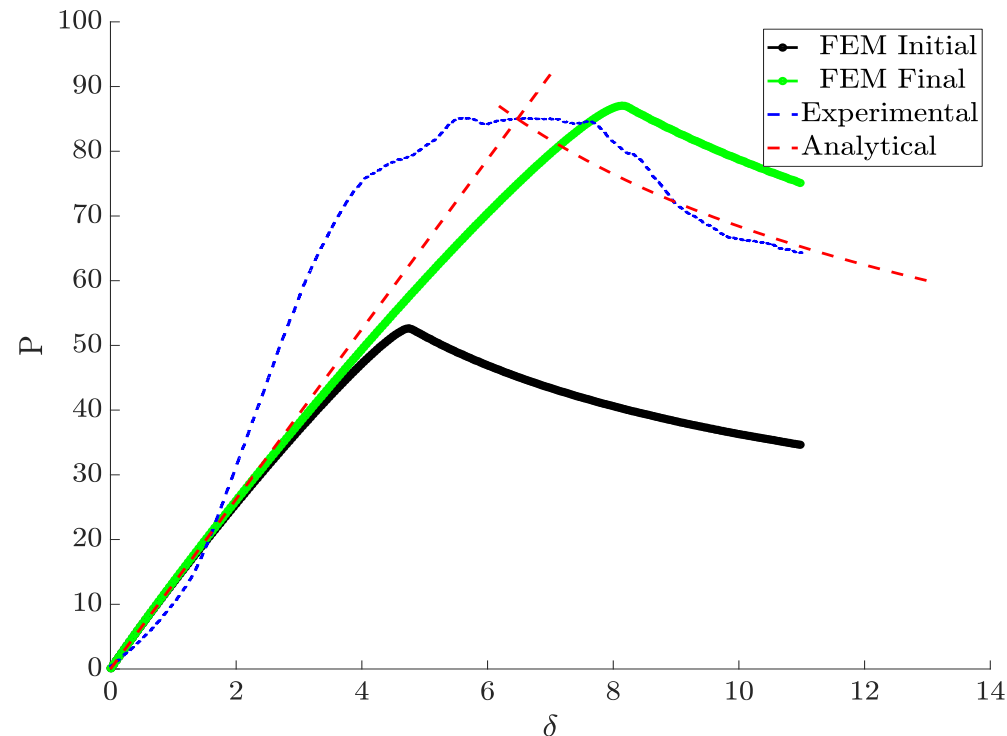
$$\phi_{n_0} = 350 \text{ N/m}, \sigma_{max} = 10 \text{ MPA}$$

Optimized Values

ϕ_n	σ_{max}
980 N/m	14.4 MPa



PRELIMINARY RESULTS



RESPONSE TO PREVIOUS YEAR REVIEW COMMENTS - SELECTIVE

- The approach is strong,...One concern area is the T-peel tests, which as correctly pointed out by the presenters is problematic (due to combined loading and asymmetry). The reviewer pointed out that shear tests or cross-tensile tests were suggested as a means to isolate shear or normal tension modes.
 - Asymmetry in T-peel test was removed by bonding backing plates on opposite sides. Similar work to isolate the shear mode is a humble recommendation of the authors for future work.
- This reviewer stated that the use of Mg/iron (Fe) impact welding to complete the molecular dynamics simulation and then apply that to the Mg/Fe ultrasonic welding (USW) process development shows great use of resources and flexibility with excellent results. Now the team just needs to do the same to Mg/Fe friction stir welding (FSW).
 - It is not trivial to make this analogy with FSW. Our project is currently conducting modeling of FSW joints using Crystal Plasticity.
- "... This reviewer is missing the plan on Mg/Fe interface by design simulation and the ongoing Mg/Fe FSW work. The reviewer strongly encouraged exploration into the other interface combinations such as supporting MAT137."
 - This is a great point; we have had interaction between IBD work and Mg/Fe FSW in previous FY and successfully helped Friction-stir Assisted Scribe joints developments. We also had interaction with MAT137 and we used adhesive joining experimental data to develop and validate the inverse DIC ZFEM modeling work.
- "... it is not clear whether interface by design will limit itself to interface strength only or if it will also include geometrical aspects. "
 - Geometrical aspects such as hook shapes during Friction-stir Assisted Scribe joining were successfully predicted by the models and validated; We investigated the geometric factors (Zn-coat thickness, coupon length) on joint strength. The Mg-Zinc eutectic is also one of the major research areas in the project FY20.
- The reviewer indicated that the slides could significantly benefit from either an overall project plan with deliverables and timing or a visual flow chart. On Slide 11 it is not clear the relative effects of lateral velocity and temperature. The reviewer asked if temperature via surface modification was pursued just because it was easier to implement.
 - Great suggestion: project flowchart added and presented. Correct to the second question: surface modification (filing) was used to obtain higher temperature because of ease of implementation. We also tried increasing lateral velocity: With 20% increase of lateral velocity (at max machine power), the peak temperature was improved by 11%.
- This reviewer said that without a clear overall picture of this project and its inter-relationship to the related process projects it is difficult to assess what the appropriate decision points are. The reviewer strongly encouraged exploration into the other interface combinations such as supporting MAT137.
 - Great suggestion: we added a slide on the overall plan with interactions between IBD and other process projects.

COLLABORATIONS, TECHNOLOGY TRANSFER, AND FUTURE WORK

► Collaborations

- ORNL and PNNL: Modeling and experimental team
- ORNL and ANL: Interface characterization of Mg/Mg and Mg/Steel
- PNNL and UT San Antonio: Development of ZFEM

► Technology Transfer

- Results will be disseminated through journal publications, conference presentations and discussions with industry
- Promising technologies will be further pursued through CRADAs with industry

► Proposed Future Work*

- ORNL – Complete phase field model with experimental validation
- ORNL – Demonstrate inverse framework on Mg/coated steel on coating thickness effects
- PNNL – Obtain and validate the adhesive parameters for an adhesive joint from the combined experimental and computational framework
- PNNL – Develop and validate a crystal plasticity-based model to predict Mg-Steel FSW joints strength

*Any proposed future work is subject to change based on funding levels

SUMMARY

- ▶ Developed and demonstrated the Interface-by-Design framework on the Mg/coated steel interface:
 - ORNL
 - Developed and validated process modeling framework for ultrasonic welding process to predict interfacial temperature
 - Developed and validated a multi-scale simulation framework for ultrasonic welding of Mg/coated steel system to predict the bond formation mechanism at the interface and bond strength/failure modes
 - Developed modal analyses framework to optimize weld spacing and coupon design for USW
 - PNNL
 - Combined modeling and experimental effort to standardize test configurations for mechanical characterization of the joints interface
 - Developed an integrated DIC ZFEM framework to inversely identify joints characteristics

FOR REVIEWERS

BACKUP SLIDES FROM HERE

TECHNICAL APPROACH

-- INTERFACE-BY-DESIGN

- Turning the equation around with validated computational models:
 - Key parameters determining the load-carrying capacity of a joint:
 - Effective bonded area, intrinsic bond strength
 - Inverse computational approach to quantify the key parameters for targeted joint load-carrying capacity:
 - Desired effective bonded area (including morphology) and bond interfacial strength
 - Perform process simulations (validated by experiments) to identify the joining methods and process parameters to achieve
 - Desired interfacial pressure, temperature history
 - Desired interfacial morphology
 - Perform massively paralleled molecular dynamics simulations validated by high resolution experiments to identify the associated interfacial characteristics needed in achieving the identified bond interfacial strength with:
 - Thermodynamics (chemistry driven) and kinetics (processing driven)
 - Diffusion and phase transformation

FY 20 PUBLICATIONS

-- ORNL

- Journal papers
 - Hui Huang, Jian Chen, Jiahao Cheng, Yong Chae Lim, Xiaohua Hu, Zhili Feng, Xin Sun. “Enhance heat generation and joint strength for ultrasonic welding of dissimilar materials AZ31 and DP590 by surface engineering”, submitted *Journal of Materials Processing Technology*, 2020.
 - Multi-Scale Characterization and Simulation of Impact Welding Between Immiscible Mg/Steel Alloys, Jiahao Cheng, Xiaohua Hu, Xin Sun, Anupam Vivek, Glenn Daehn, David Cullen, accepted *Journal of Materials Science & Technology*, 2020.
 - Molecular Dynamics Study on Microstructure and Bonding Strength of Impact-Welded Mg-Steel Joints, Jiahao Cheng, Xiaohua Hu, Xin Sun, submitted *Computational Materials Science*, 2020.
 - Synchrotron experiment and simulation studies of magnesium-steel interface manufactured by impact welding, Lianghua Xiong, Andrew Chuang, Jiahao Cheng, Xiaohua Hu, Dileep Singh, Xin Sun, in preparation.
- Conference presentations
 - Hui Huang, Jian Chen, Yong Chae Lim, Zhili Feng, Xin Sun. ‘Enhance Heat Generation and Joint Strength in Dissimilar Metal Ultrasonic Welds by Surface Engineering’, AWS annual professional program, Nov 11-14, 2019, Chicago, IL
 - Multi-Scale Study Of Bonding Mechanism Between Immiscible Mg/Steel Alloys, Jiahao Cheng, Xiaohua Hu, Xin Sun, Anupam Vivek, Glenn Daehn, David Cullen, Minerals, Metals, and Materials (TMS) Annual Meeting & Exhibition 2020, February 2020 | San Diego, CA
 - Synchrotron x-ray diffraction and computed tomography studies of ultrasonic welding dissimilar Mg-Fe metals, Lianghua Xiong, Andrew Chuang, Dileep Singh, Jian Chen, Yong Chae Lim, Zhili Feng, Minerals, Metals, and Materials (TMS) Annual Meeting & Exhibition 2020, February 2020 | San Diego, CA

FY 20 PUBLICATIONS

-- PNNL

- Wang T., D. Ramirez Tamayo, X. Jiang, P. Kitsopoulos, W. Kuang, V. Gupta, and E.I. Barker, et al. 2020. "Effect of interfacial characteristics on magnesium to steel joint obtained using FAST." Materials & Design 192, no. 2020:108697.
- Shank S. Kulkarni, Varun Gupta, Angel Ortiz, Hrishikesh Das, Piyush Upadhyay, Erin Barker, Darrell Herling, "Determining cohesive parameters for modeling inter-facial fracture in dissimilar friction stir welded joints" submitted International Journal of Solids and Structures, 2020.
- Daniel Ramirez-Tamayo, Varun Gupta, Arturo Montoya, Ethan Nickerson, Timothy Roosendaal, Kevin Simmons, Gayaneh Petrossian, and Harry Millwater "A Complex-variable Finite Element Method-based Inverse Methodology to Extract Constitutive Parameters" in preparation, 2020.